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Molecular dynamics simulation study of cold spray process

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ABSTRACT

Cold Spray (CS) process is a deposition process in which micron-to-nano sized solid particles are deposited on a substrate using high-velocity impacts. Unlike thermal spray processes, CS process does not melt the particles thus retaining their original physical and chemical properties. These characteristics make CS process ideal for various engineering applications. The bonding mechanism involved in CS process is hugely complicated considering the dynamic nature of the process. Even though CS process offers great promises, the realization of its full potential is limited by lack of understanding of the complex mechanisms involved. The study focuses on understanding the complex nanoscale mechanisms involved in CS process. The study uses Molecular Dynamics (MD) simulation technique to understand the material deposition phenomenon during the CS process. For the simulation conditions used, the study finds that the quality of deposition is highest for an impact velocity of 700 m/s, the particle size of 20 Å and an impact angle of 90°. The von Mises stress and plastic strain analysis revealed that bonding mechanism in CS process could be attributed to adiabatic softening, adiabatic shear instabilities followed by interfacial jetting of particle materials resulting in a uniform coating. The findings of this study can further the scope and applications of CS process.

1. Introduction

Cold Spray (CS) is an emerging solid-state deposition process, where micron-to-nano sized particles bond to a substrate due to high-velocity impact. Unlike thermal spray processes, chemical and physical properties of deposited particles are retained in CS process considering the solid-state low-oxidized nature of the coating. These characteristics make CS process ideal for several critical engineering applications in industries such as defense and aerospace sectors [1]. During CS process, the acceleration of particles is achieved by the expansion of hot pressurized gases through a converging-diverging nozzle [2]. The high-velocity impact of the accelerating particles causes plastic deformation of the particles and the substrate surface resulting in a uniform coating. The schematic of CS process is shown in Fig. 1. The quality of the coating during the CS process is influenced by the incident velocity of the particles [1]. The successful bonding of powder particles on the substrate occurs only when the velocity of sprayed material exceeds a critical value that is specific to the material [1]. For instance, the critical velocity is found to be approximately 570 m/s for copper particles having a size of 5–25 μm [3].

The material suitability for CS process depends on the mechanical and physical properties including material hardness, melting temperature and density [4]. Materials with relatively low yield strength such as copper, aluminum, and zinc are considered ideal for the CS process as they exhibit relatively high softening at elevated temperatures [5]. High strength materials are not ideal for CS process as they do not provide enough energy for deposition [6]. Experimental study on CS process of metal particles on polymer reveals that no metal particles can be coated on soft polymer due to lack of plastic deformation of particles [7]. Other factors influencing the quality of deposition during CS process include angle of impact, gas flow rate and stand-off distance between the nozzle tip and target surface [8]. Study on variations in stand-off distances (range 10 mm–110 mm) for particles of aluminum, titanium and copper powders showed deposition efficiency decreases with increase in stand-off distance [9]. Most of the studies reported on CS process is performed through experimentation [10]. While experimental techniques reveal the quality of material deposition and the microstructural characteristics, the use of experimentation in understanding dynamic mechanisms involved in the CS process is often limited.

Simulation tools such as finite element (FE) simulation techniques and numerical methods have often been used as an alternative way in these cases. FE simulation have been used to understand the effect of process parameters during CS and other thermal spray processes at macroscales. The impact dynamics, bonding mechanism, and critical velocities during the CS process were studied using FE simulation tool ABAQUS [6]. The study found that the critical velocity depends on several parameters including the type of spray material, powder

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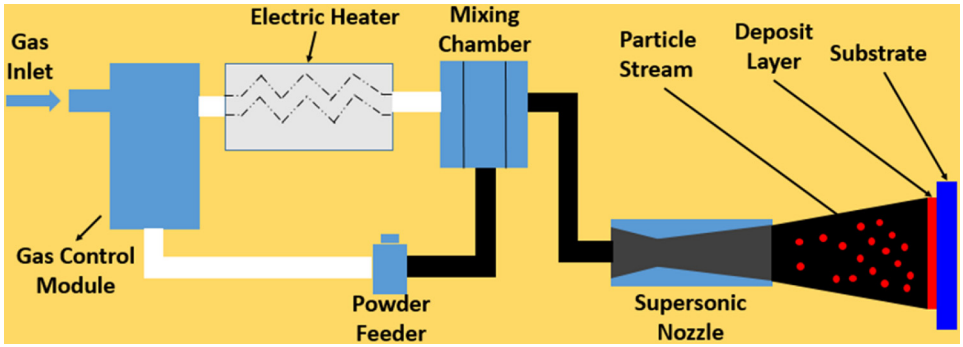

Fig. 1. Schematic of Cold Spray Process.

quality, particle size and the particle impact temperature. Splat formation during the thermal process was studied by numerical simulation method which revealed that increase in substrate temperature reduces the formation of splats [11]. FE tool ABAQUS/Explicit used for simulation study on CS process showed that a minimal impact particle velocity needed to produce shear localization [12]. It is known that the feed powder particles and the substrate and deposited material (after the first layer of particle impact) suffer a full localized distortion during impact. It causes disturbance of the thin surface films forming an adiabatic shear band which enables a conformal interaction between the particles and the substrate/deposited material. Formation of high strain rates during impact along with continuous deformation on the shear band leads to instability which causes the material to behave as a liquid material although in a solid-state. This close interaction of clean surfaces combined with high contact pressures is supposed to be the necessary circumstances for particles/substrate and particle/particle bonding. This phenomenon is unique and leads to a strong bond between parent material and the impacting particle.

It is agreed that the actual mechanism when solid particles deform and bond onto the substrate during cold spray is still not well understood [12]. FE simulation studies are not capable of explaining the bonding process accurately. Because bonding during the CS process happens at molecular scale, Molecular Dynamics (MD) simulation technique is considered as the ideal tool. During MD simulation, the movements and interactions of atoms or molecules are determined based on the classical equations of motion. However, very few studies have reported on the use of MD simulation on CS process thus far [13]. One such study has used MD simulation to understand the effect of impact velocity on coating process of titanium and nickel particles on titanium substrate during CS process [13]. The study revealed that higher impact velocities result in the stronger interface between the particle and substrate. MD simulation has also been used to investigate structure-property relation during thermal spray processes [14]. The study found that maximum diameter after the impact and the height of the splat increases with increasing Reynolds number of the flow stream until a critical value is reached.

From the literature review, it is evident that the effect of critical process parameters on the bonding and the real complex phenomenon of particle/substrate and particle/particle bonding during the CS process is not understood at the nanoscale. This study focusses on the use of molecular dynamics simulation investigate the bonding mechanism in CS process and to understand the effect of critical parameters including impact velocity, particle size and angle of impact on the material deposition phenomenon during the CS process of copper nanoparticles on the copper substrate. The effect of parameters including particle shape, material type and properties, and particle concentration are not considered in this study.

2. MD simulation

In the current study, the simulation of CS process is performed using "Large-scale atomic/molecular massively parallel simulator" (LAMMPS) [15]. The study considers the impact of nanoparticle impact on the surface of a metal substrate in three-dimension (3D). The simulation system consists of copper (Cu) atoms as a substrate, and a nanoparticle also made of Cu atoms. The substrate is made of 30,000 atoms of Cu, and the nanoparticle is made of 100 Cu atoms in fcc lattice structure. The shape of the substrate is a rectangular block having dimensions of 100 Å × 100 Å × 20 Å with face-centered cubic (fcc) lattice structure having a lattice spacing of 3.61 Å. The nanoparticle is spherical having a diameter of 10 Å with Cu atoms arranged in (fcc) lattice structure having a lattice spacing of 3.61 Å. The schematic of the model used for CS process simulation is shown in Fig. 2.

The conditions used for CS process simulation study are given in Table 1. The interatomic forces between the Cu-Cu atoms are calculated using Embedded Atom Method (EAM), a suitable potential for the simulations of structural, mechanical, and thermal properties of metallic systems including Cu [16]. The Velocity-Verlet algorithm is employed to calculate the position and velocity of the atoms. In the actual working of CS, particles of varying shapes and sizes strike randomly on the substrate surface. The present MD simulation study considers only a single impact of a particle on the substrate under varying operational conditions. It is assumed that a single impact of a particle can explain the complex bonding mechanism involved in the CS process. Embedded Atom Method model function for the fcc of copper and its alloys [16]. In the computational simulation, the potential energy of an atom, i is given by

$$E_i = F\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\Phi\alpha\beta r_{ij} \quad (1)$$

where i and j $(i \neq j)$ label the atoms in the solid, r_{ij} is the distance between atoms i and j, and ρ_β is the electron density at the position of atom i due to all other atoms in the solid. It is supposed that this density can be given as a sum of individual atomic densities $f(r_{ij})$ where r_{ij} is the distance between i atoms j, $\Phi_{\alpha\beta}$ and is a potential function, ρ_β is the

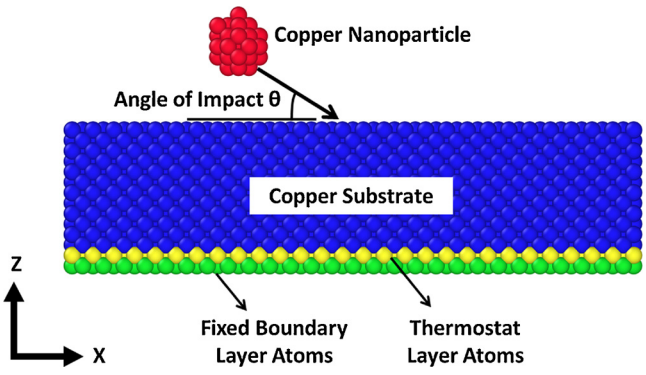

Fig. 2. Schematic of MD Simulation Model of Cold Spray Process.